

## Thermodynamic functions of lactams in the ideal gas state

Emel'Yanenko V., Turovtsev V., Orlov Y.

Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

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### Abstract

Thermodynamic functions (enthalpy, entropy, free energy, and heat capacity) of azacycloalkan-2-ones with ring sizes  $n = 4-8$  in the ideal gas state are calculated by means of quantum chemistry and statistical physics, using an anharmonic approximation in the range of 298-1500 K with allowance for all known conformers and optical isomers. Equilibrium structures and total energies of lactams are calculated using the B3LYP/6-311++G(3df, 3pd), B3LYP/aug-cc-pVQZ, and MP2/6-311++G(3df, 3pd) methods, and the anharmonic frequencies of the fundamental vibrations of all the investigated structures were found via B3LYP/6-311++G(3df, 3pd). © 2014 Pleiades Publishing, Ltd.

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### Keywords

anharmonic frequencies, enthalpy of formation, entropy, Gibbs free energy, heat capacity, lactams, rigid rotator-anharmonic oscillator, thermodynamic properties